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# Radiation Diffusion in NIF-ALEAMR

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Livermore, CA, Afghanistan
June 2, 2008 through June 4, 2008

# Radiation Diffusion in NIF-ALEAMR

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QuickTime™ and a
Photo - JPEG decompressor
are needed to see this picture.

3rd International Workshop on High-Powered Laser Chamber Issues

Livermore, CA

June 2-4, 2008

**Lawrence Livermore National Laboratory, P. O. Box 808, Livermore, CA 94551**

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# Outline

- Governing equations
- Discretization
- Operator split implementation
- Poisson solver implementation
- Testing
- Mix cell support
- Results for key hole design
- NIF-ALEAMR application modules
- Summary

# Radiation diffusion governing equations

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- Radiation and material energy equations

Radiation energy equation

$$\frac{\partial E_R}{\partial t} = \nabla \cdot \left( \frac{c\lambda(E_R)}{\kappa_R} \nabla E_R \right) + \kappa_P \left( 4\sigma T^4 - cE_R \right)$$

Material energy equation

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\mathbf{u}\rho E + \mathbf{u}p) = 0 - \kappa_P \left( 4\sigma T^4 - cE_R \right)$$

Energy transfer towards equilibrium between material and radiation temperature

- New variable $E_R$ is radiation energy
  - Governed by nonlinear diffusion equation
- Nonlinear opacities $\kappa_P(\rho,T)$ *and* $\kappa_R(\rho,T)$
- Flux limiter $\lambda(E_R)$ is used to limit propagation speed

# Operator split integration

- Hydro update without radiation

$$(\rho E)^{-} = (\rho E)^{n} - \Delta t\left[\nabla \cdot \left(\mathbf{u}\rho E + \mathbf{u}p\right)\right]^{n+1/2}$$

- Hydro update is followed by backward-Euler energy/radiation update

$$\frac{E_R^{n+1} - E_R^{n}}{\Delta t} = \nabla \cdot \left( \frac{c\lambda\left(E_R^{n+1}\right)}{\kappa_R^{n+1}} \nabla E_R^{n+1} \right) + \kappa_P^{n+1}\left(B^{n+1} - cE_R^{n+1}\right)$$

$$(\rho E)^{n+1} = (\rho E)^{-} - \Delta t \kappa_P^{n+1}\left(B^{n+1} - cE_R^{n+1}\right)$$

- Operator split approach lets radiation diffusion plug in as a module

# Nonlinear equation solver uses Newton Iterations

- Nonlinear equations for the backward Euler updates:

$$F_\alpha = (\rho e)^{n+1} - (\rho e)^{-} + \Delta t \kappa_p \left(B^{n+1} - cE_R^{n+1}\right) = 0$$

$$F_R = E_R^{n+1} - E_R^{n} - \Delta t \nabla \cdot \left(D^{n+1} \nabla E_R^{n+1}\right) + \kappa_P^{n+1}\left(B^{n+1} - cE_R^{n+1}\right) = 0$$

- Corrections $\delta Q_\alpha$, $\delta E_R$ in the Newton iterations satisfy:

$$\begin{bmatrix} \frac{\partial F_\alpha}{\partial Q_\alpha} & \frac{\partial F_\alpha}{\partial E_R} \\ \frac{\partial F_R}{\partial Q_\alpha} & \frac{\partial F_R}{\partial E_R} \end{bmatrix} \begin{bmatrix} \delta Q_\alpha \\ \delta E_R \end{bmatrix} = \begin{bmatrix} -F_\alpha \\ -F_R \end{bmatrix}$$

$$(\rho e)_\alpha \leftarrow (\rho e)_\alpha + \delta Q_\alpha$$

$$E_R \leftarrow E_R + \delta E_R$$

- Invert diagonal upper left block matrix (Schur complement):

$$\begin{bmatrix} \frac{\partial F_\alpha}{\partial Q_\alpha} & \frac{\partial F_\alpha}{\partial E_R} \\ 0 & \frac{\partial F_R}{\partial E_R} - \frac{\partial F_R}{\partial Q_\alpha}\left(\frac{\partial F_\alpha}{\partial Q_\alpha}\right)^{-1} \frac{\partial F_\alpha}{\partial E_R} \end{bmatrix} = \begin{bmatrix} \delta Q_\alpha \\ \delta E_R \end{bmatrix} = \begin{bmatrix} -F_\alpha \\ -F_R + \frac{\partial F_R}{\partial Q_\alpha}\left(\frac{\partial F_\alpha}{\partial Q_\alpha}\right)^{-1} F_\alpha \end{bmatrix}$$

# Poisson solver implementation

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$$\nabla \cdot \left( D(\phi) \nabla E_R \right) = S$$

- Cell-centered $E_R$, $\kappa_R$, $\kappa_P$ and diffusion coefficients on deformed mesh. Colocating $T$, and $E_R$ avoids spurious diffusion from to interpolation.
- Discretization:
  - Conservative finite difference due to Henshaw, SIAM J. Sci. Comp., Vol. 28, pp. 1730-1765.
  - 9-point stencil in 2D. 27-point in 3D. Formally second order accurate on smooth mesh.
  - Supports discontinuous coefficient. Using linear or harmonic average of $D$ at cell interfaces.
  - Symmetric, except for boundary conditions
- Hypre preconditioner

# Flux Limiting

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- Flux limiting is generally needed for thin media, to prevent waves from exceeding the speed of light. In practice, limiting is ad hoc.
- Diffusion coefficient $D=c\,\lambda(E_R)/\kappa_R$ contains nonlinear factor $\lambda(E_R)$
- Unlimited flux: $\lambda(E_R)=\frac{1}{3} \qquad D=\frac{c}{3\kappa_R}$
- Levermore-Pomraning formula based on Chapman-Enskog theory

$$\lambda(R)=\frac{1}{R}\left(\coth(R)-\frac{1}{R}\right) \qquad R\sim\left|\frac{\nabla E}{E}\right|$$

- Larson limiter formula:

$$D=\frac{c}{\sqrt[n]{\left[(3\kappa_R)^n+\left|\frac{\nabla E}{E}\right|^n\right]}}$$

# NIF-ALEAMR code combines problem-specific routines with SAMRAI components

NIC
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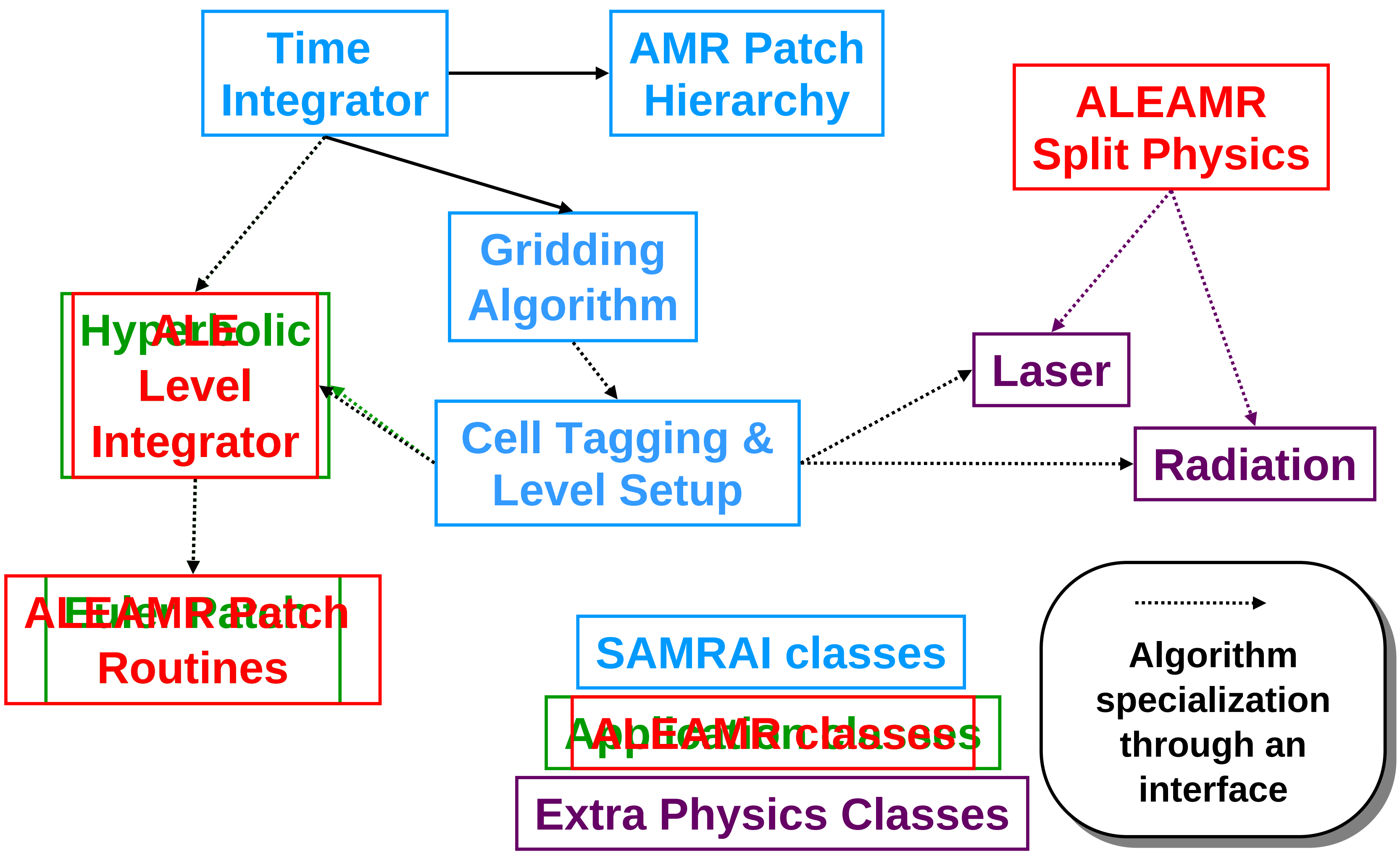

# Split physics interface in ALEAMR

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```
SplitPhysics
initialize();
preHierarchyAdvanceHook();
postHierarchyAdvanceHook();
postRegridHook();
getNextDt();
tagCells();
```

```
RadiationDiffusionPhysics
initialize();
preHierarchyAdvanceHook();
postHierarchyAdvanceHook();
postRegridHook();
getNextDt();
tagCells();
```

Apply radiation physics effects

```
do {
  physics->preHierarchyAdvanceHook(…);

  // update hydro
  next_dt = …;

  physics->postHierarchyAdvanceHook(…);
  next_dt = min(next_dt, physics->getNextDt());
} while ( time < final_time );
```

# Testing of radiation diffusion solver

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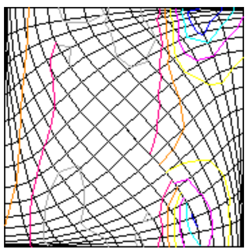
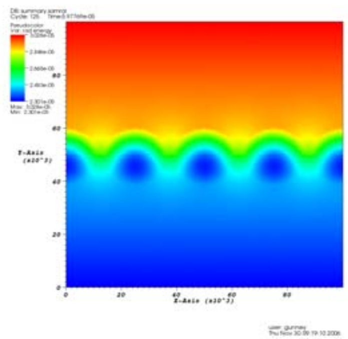
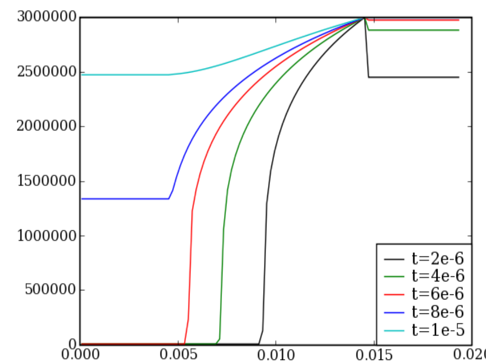
- Poinsson solver test
- Second order accurate for smooth coefficients.
- First order accurate with disontinuous coefficients



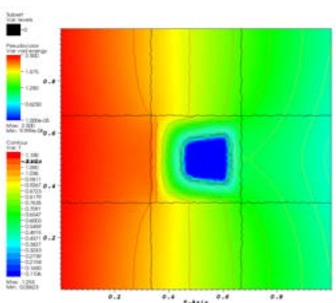
- Linear diffusion on randomized mesh with discontinuous coefficients



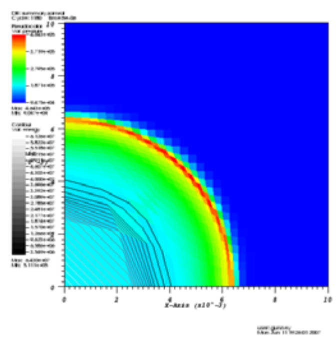
- 1D nonlinear Marshak wave with multimaterial




- 2D nonlinear Marshak wave with multimaterial



- LEOS and rad-hydro integration



- Currently testing mix cell support and solver robustness

# Poisson solver verification on randomized mesh

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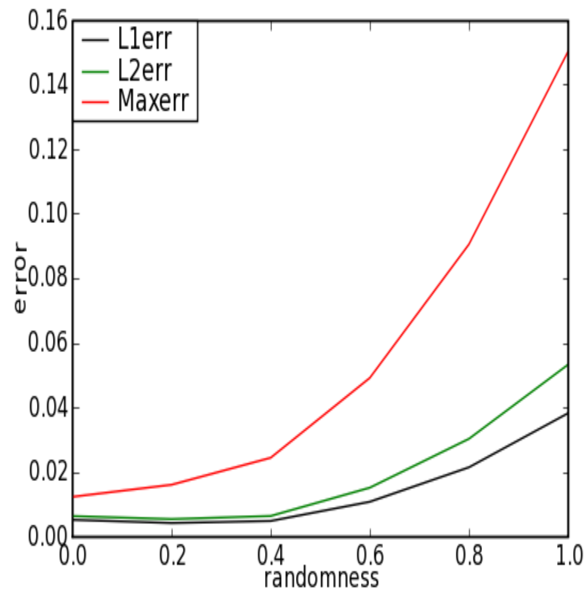
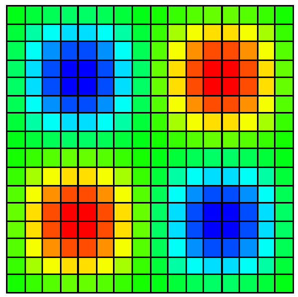
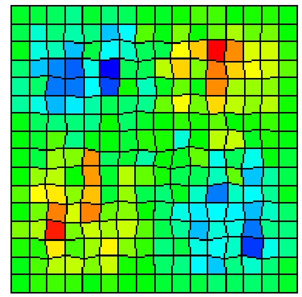
- Div(grad(u)) = sin(x)sin(y)
- Dirichlet boundary conditions
- L2 error norms showed

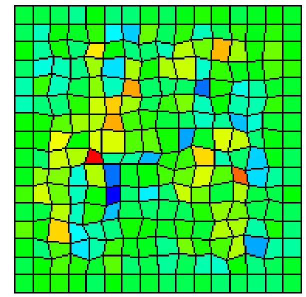


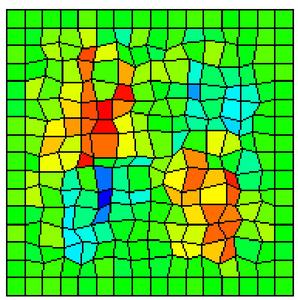
**Randomness = 0**



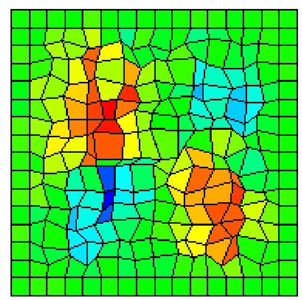
**Randomness = 2**



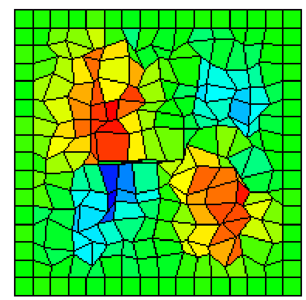
**Randomness = 4**



**Randomness = 6**



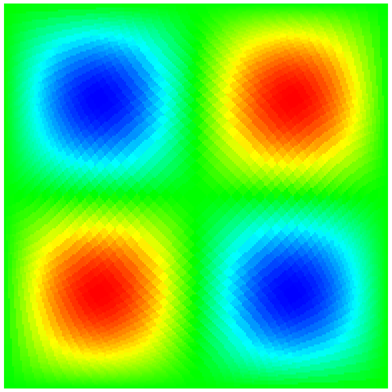
**Randomness = 8**



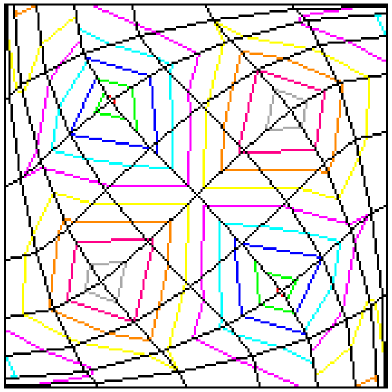
**Randomness = 10**

# Poisson solver verification on twisted mesh

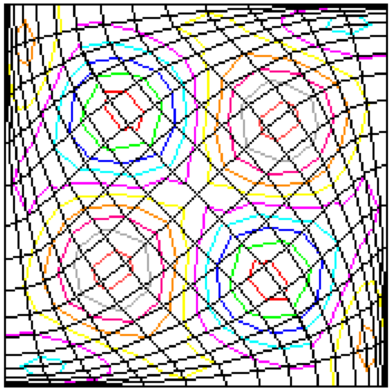
- Div(grad(u)) = sin(x)sin(y)
- Dirichlet boundary conditions
- Second order accurate



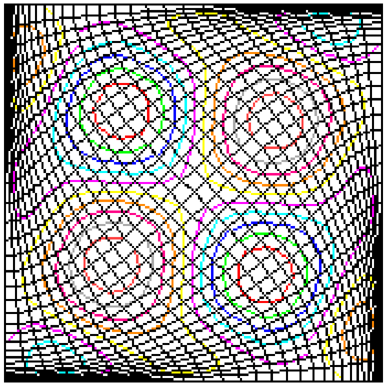
Exact solution



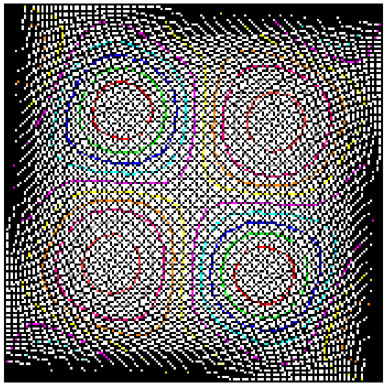
8x8 grid, error = .0555



16x16 grid, error = .0130



32x32 grid, error = .0032



64x64 grid, error = .0008

# Poisson solver verification on twisted mesh, with discontinuous coefficients

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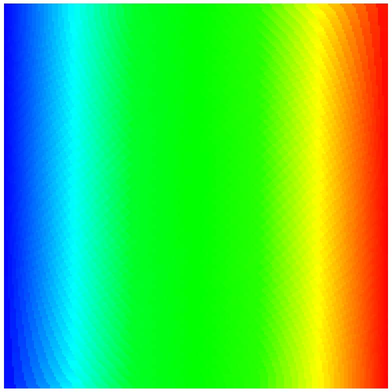
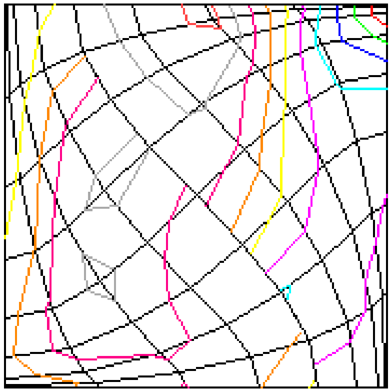
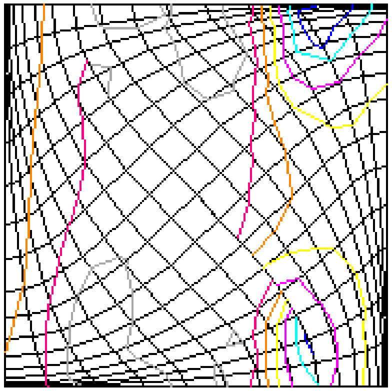
- Div(grad(u)) = 0
- Diffusion coefficients 1 and 1000
- L2 error norms shown
- First order accurate with disontinuous coefficients



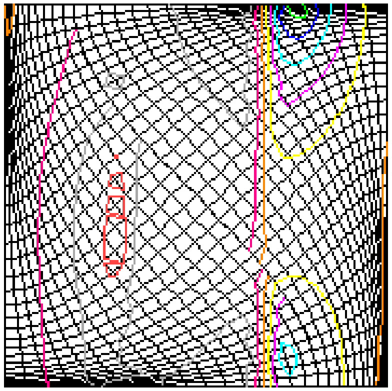
Exact solution



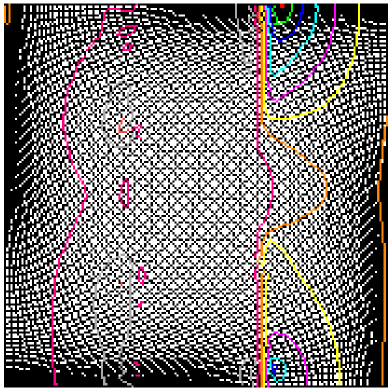
8x8 grid, error = .0944



16x16 grid, error = .0367



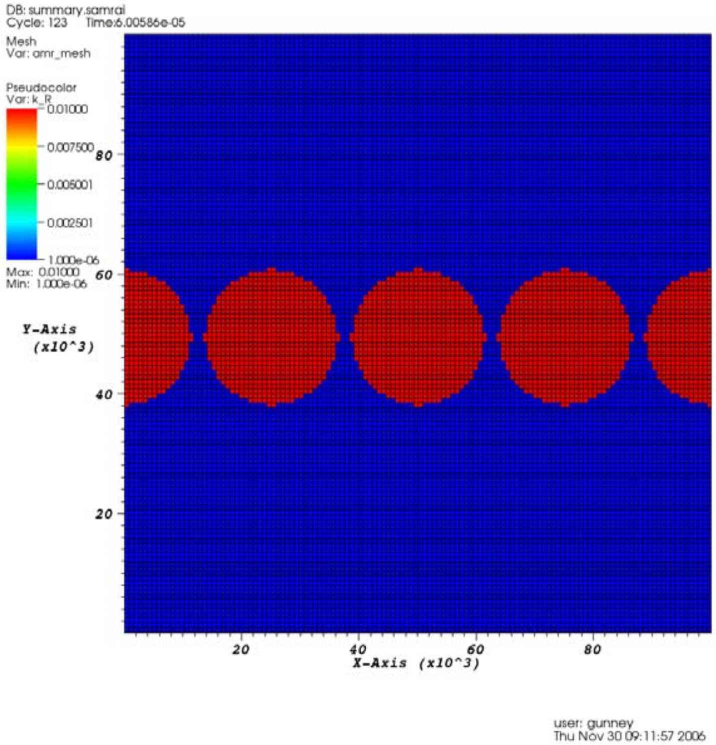
32x32 grid, error = .0184



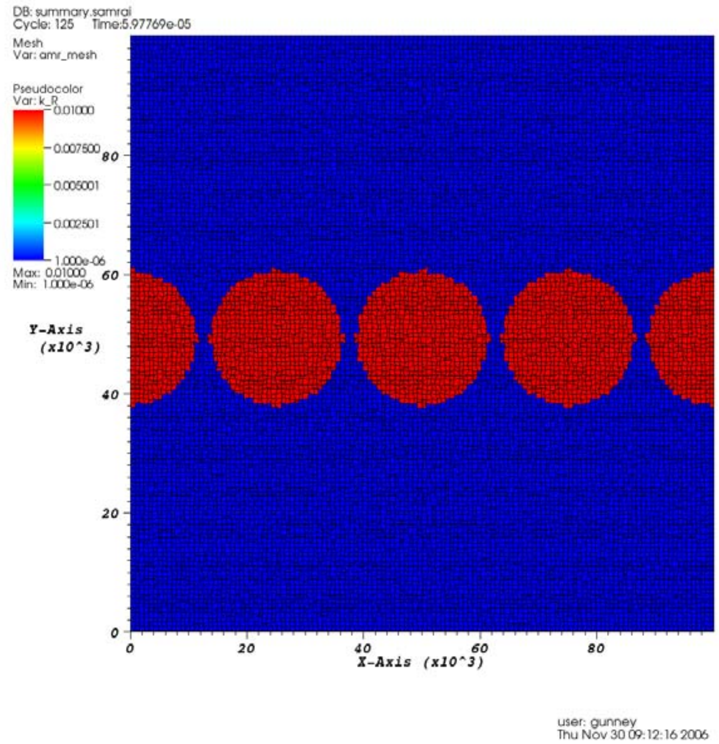
64x64 grid, error = .0090

# Cloud problem definition

## Cartesian grid




## Randomized grid




- $\kappa_P=0$
- $\kappa_R=10^{-6}$ for air, $\kappa_R=10^{-2}$ for clouds
- Incoming flux at top

# Cloud problem results: mesh randomness does not degrade accuracy

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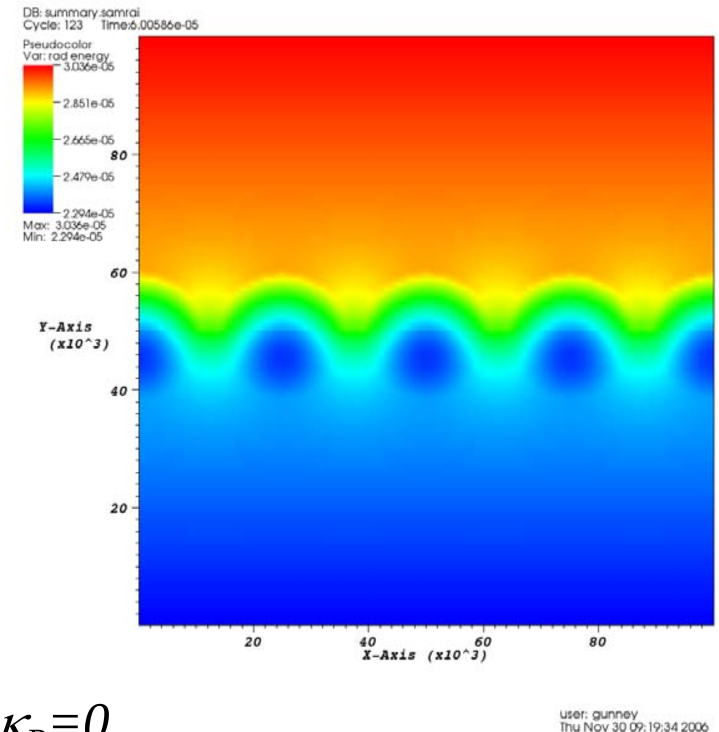
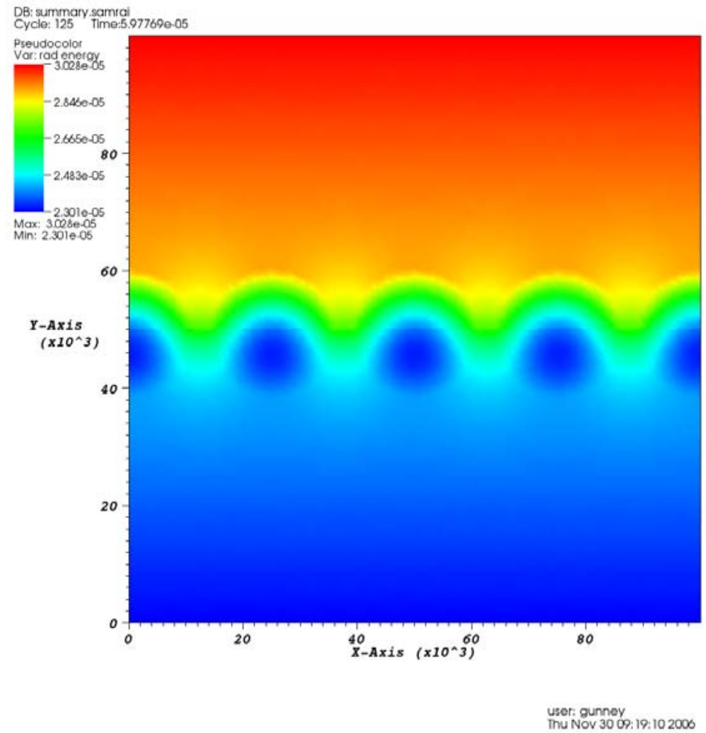
**Cartesian grid**




**Randomized grid**




- $\kappa_P=0$
- $\kappa_R=10^{-6}$ for air, $\kappa_R=10^{-2}$ for clouds
- Incoming flux at top

# 1D thermal wave test problem

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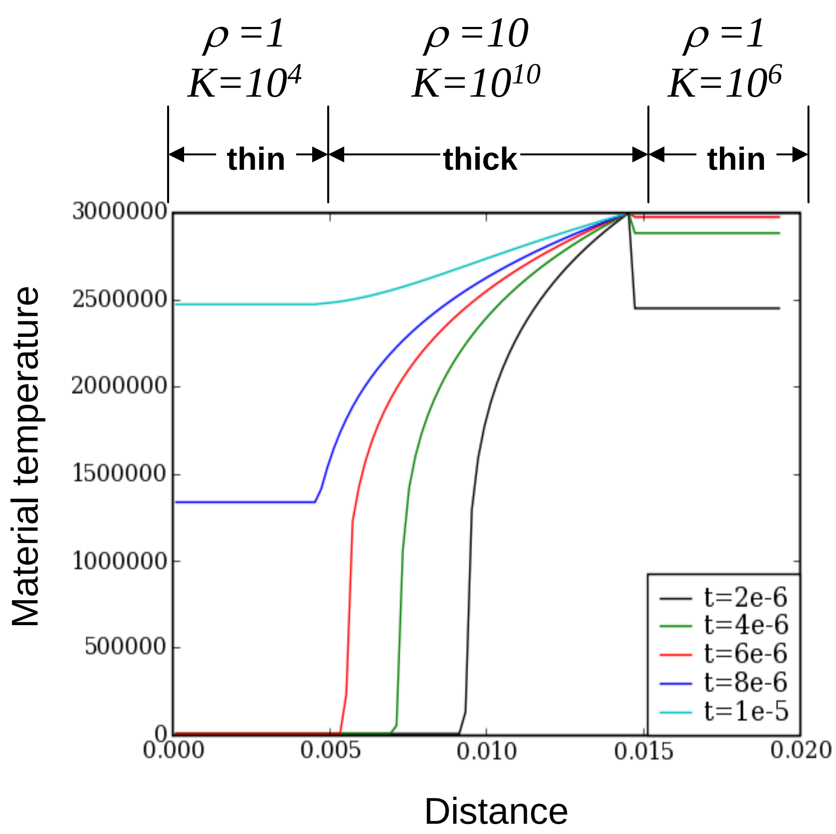
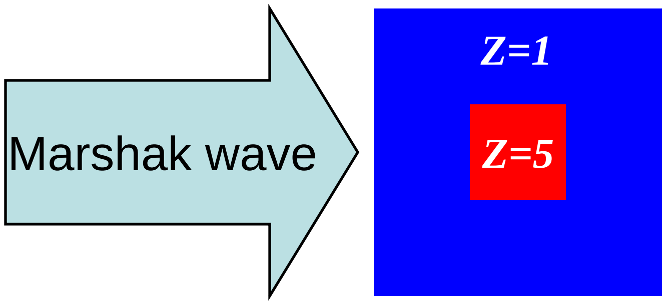
- From Howell and Greenough, JCP Vol. 184, pp. 53-78.
- Marshak wave from right burns through optically thick center slab.
- Radiation temperature of 3,000,000 imposed on right side.
- $\kappa_R = \kappa_P = K\rho^2/T$
- Low density right side heats up quickly from radiation.
- Left side initially protected by center slab.
- Low density left side heats up quickly after center slab burns away.
- Uniform mesh

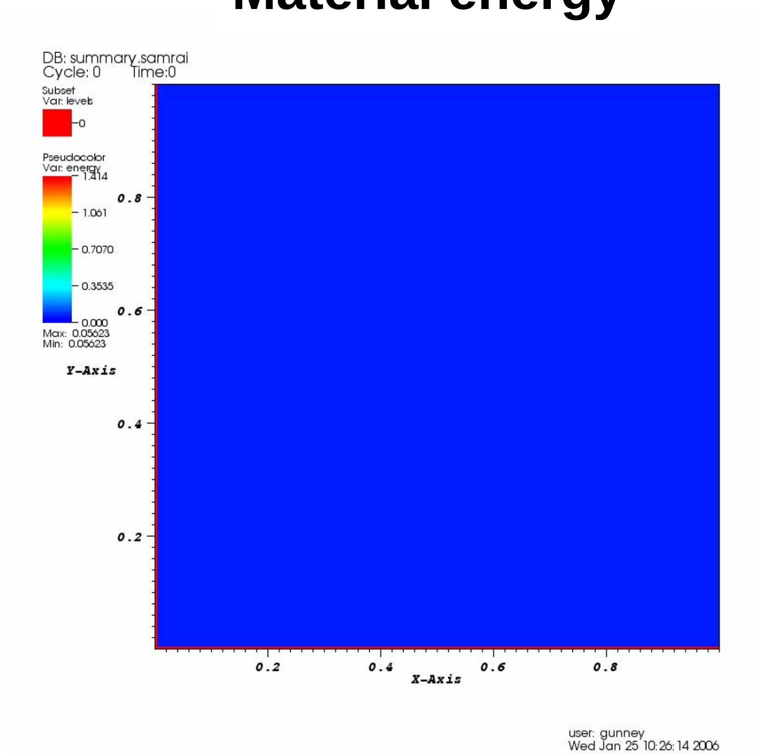


# 2D Mousseau problem

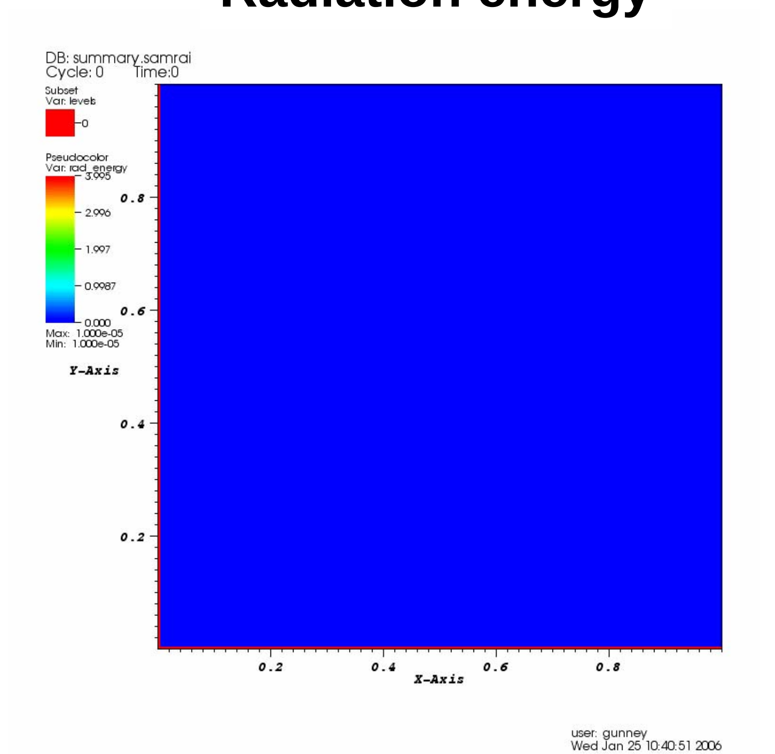



- Mousseau, et al., JCP, Vol. 160, pp. 743-765, 2000.
- $D_r(T) = (T/Z)^3$
- Nonlinear high and low Z materials.
- Marshak wave enters at left

## Material energy

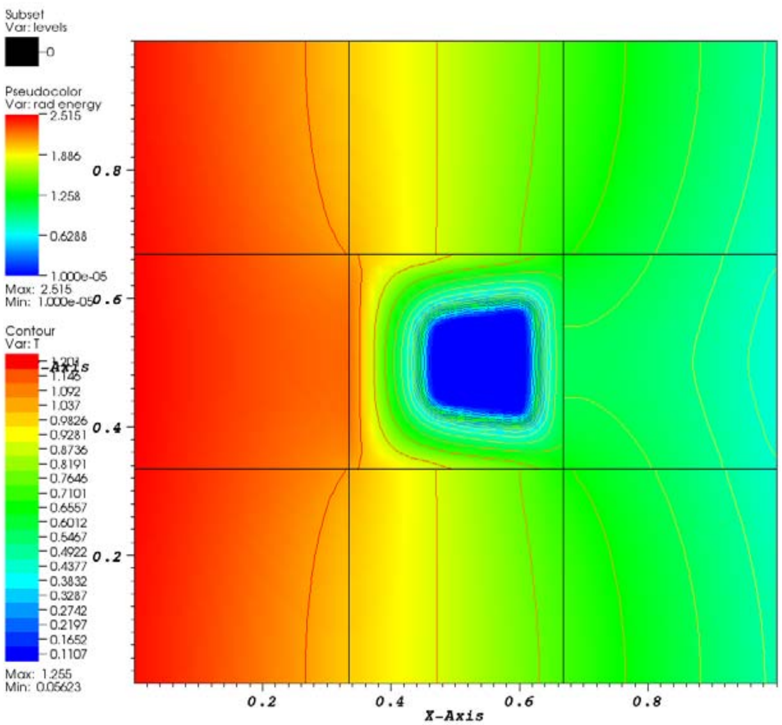



## Radiation energy

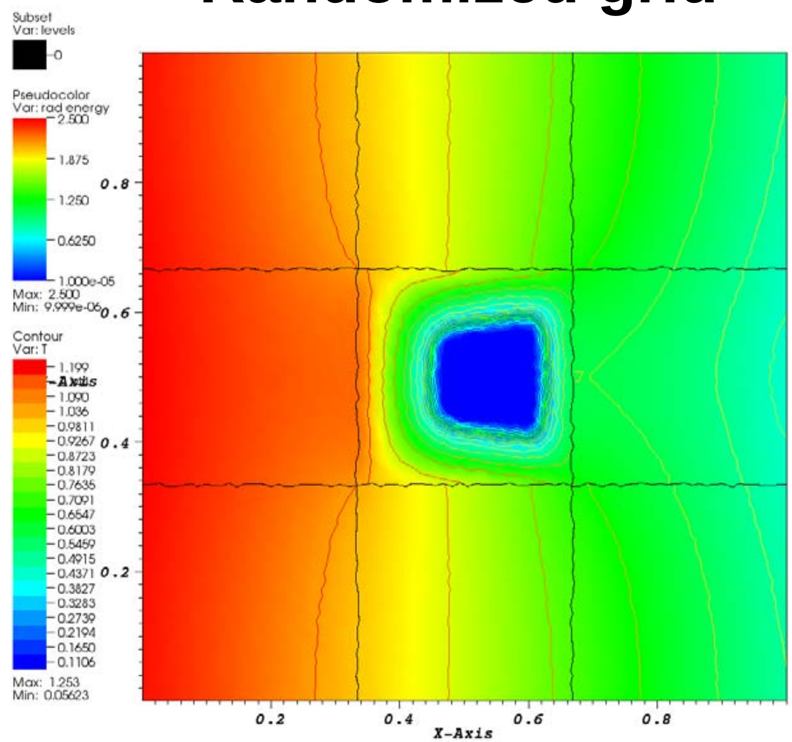


# 2D Mousseau results: radiation energy, material T on Cartesian and randomized grids

## Cartesian grid

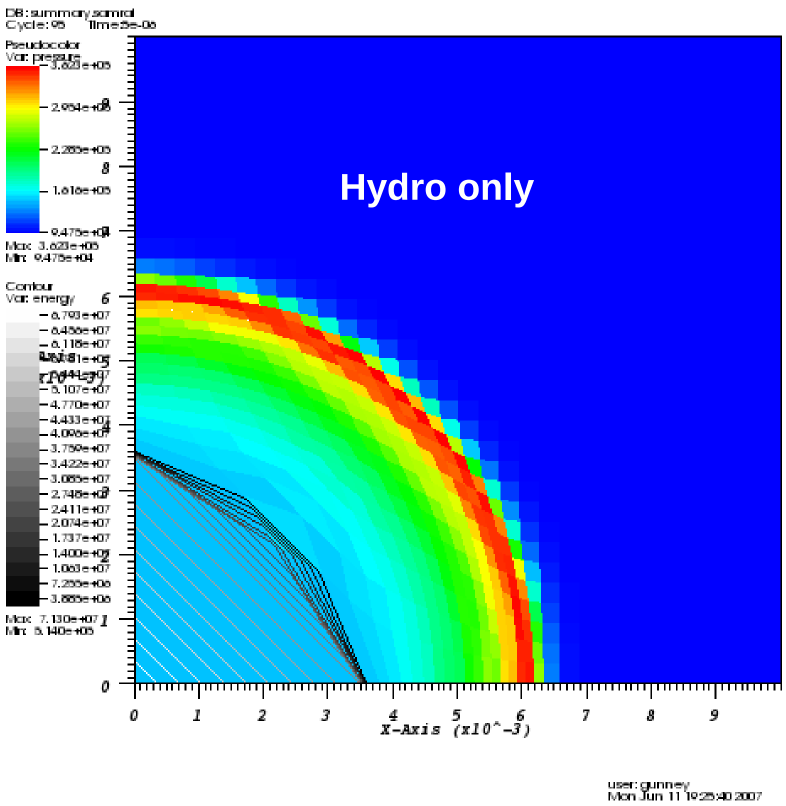


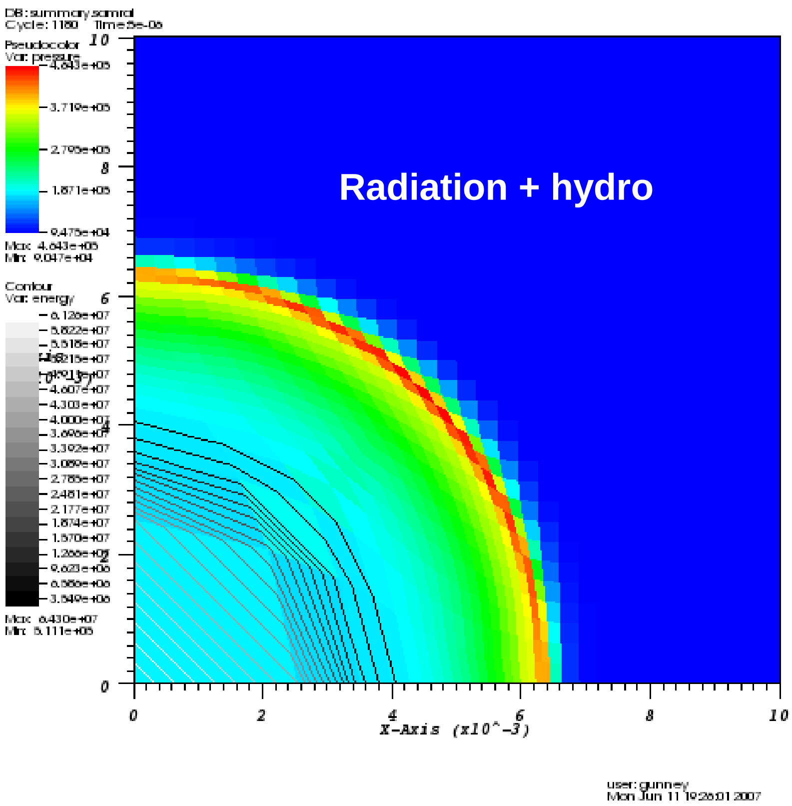

## Randomized grid



# Coupled radiation hydro results

- Sedov problem: Initial energy input at corner sends out cylindrical shock wave
- Air, heated to 30,000K
- Tabulated equation of state
- Color = pressure, contour lines = material energy



# Rad Diffusion with Mix Cell data

- Multiple materials occupying one cell, with associated cell volume fractions $f_\alpha$.

$$\frac{\partial}{\partial t}(\rho E)_\alpha + \nabla \cdot \left(\mathbf{u}(\rho E)_\alpha + \mathbf{u} p_\alpha\right) = -f_\alpha \kappa_{P,\alpha}\left(4\sigma T_\alpha{}^4 - cE_R\right)$$

$$\frac{\partial E_R}{\partial t} = \nabla \cdot \left(\frac{c\lambda(E_R)}{\kappa_R}\nabla E_R\right) + \sum_\alpha f_\alpha \kappa_{P,\alpha}\left(4\sigma T_\alpha{}^4 - cE_R\right)$$

- Cell-averaged Rosseland opacity

$$\kappa_R = \frac{\sum_\alpha f_\alpha \rho_\alpha \kappa_{R,\alpha}}{\sum_\alpha f_\alpha \rho_\alpha}$$

- Averaging for interface diffusion coefficients

$$D = \frac{D_r + D_l}{2} \qquad\qquad D = \frac{2D_r D_l}{D_r + D_l}$$

# 2D Analysis of Key Hole under Radiative Heating

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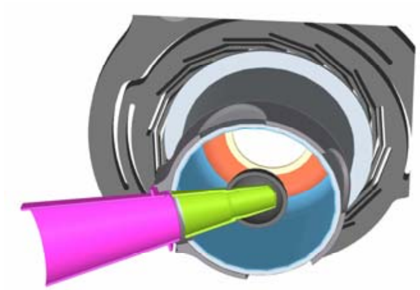
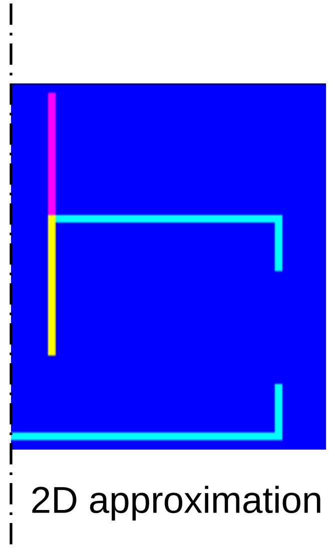
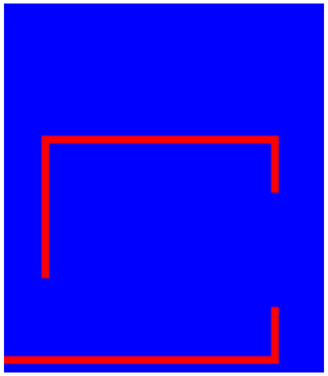


Key Hole



2D approximation



Initial temperature distribution

- 0.2mm aluminum Hohlraum walls
- 0.2mm aluminum inner and outer cone walls
- Initial temperatures of 0.1, 0.2 and 0.3 keV for inner cone and Hohlraum wall

# Summary

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- Radiation diffusion solver supporting ALE mesh, multi-material with mix cells.
- Future work:
  - Further testing and validation on rad-hydro fragmentation problems.
  - AMR version.